

Nonsinusoidal current–phase relation in SFS Josephson junctions

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Various types of the current–phase relation $I(\varphi)$ in superconductor–ferromagnet–superconductor (SFS) point contacts and planar double-barrier junctions are studied within the quasiclassical theory in the limit of thin diffusive ferromagnetic interlayers. The physical mechanisms leading to highly nontrivial $I(\varphi)$ dependence are identified by studying the spectral supercurrent density. These mechanisms are also responsible for the $0-\pi$ transition in SFS Josephson junctions.

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The relation between the supercurrent I across a Josephson junction and the difference φ between the phases of the order parameters in the superconducting banks is an important characteristic of the structure. The form of $I(\varphi)$ dependence is essentially used for analyzing the dynamics of systems containing Josephson junctions [1]. Studying $I(\varphi)$ also provides information on pairing symmetry in superconductors [2].

In structures with tunnel-type conductivity of a weak link (SIS) the current–phase relation is sinusoidal, $I(\varphi) = I_c \sin \varphi$ with $I_c > 0$, in the whole temperature range below the critical temperature. At the same time, in point contacts (ScS) and junctions with metallic type of conductivity (SNS) strong deviations from the sinusoidal form take place at low temperatures T [3] with the maximum of $I(\varphi)$ achieved at $\pi/2 < \varphi_{\max} < \pi$.

The situation drastically changes if there is magnetoactive material in the region of weak link. The transition from the 0-state [$I(\varphi) = I_c \sin \varphi$ with $I_c > 0$] to the π -state ($I_c < 0$) in junctions containing ferromagnets has been theoretically predicted in a variety of Josephson structures [4, 5, 6, 7, 8, 9, 10, 11, 12] and experimentally observed in SFS and SIFS junctions [13, 14]. In the general case modifications of $I(\varphi)$ do not reduce to the $0-\pi$ transition. It was shown that tunneling across ferromagnetic insulator (F_I) in clean $SF_I S$ junctions [15] or across a magnetically active interface between two superconductors [16] may result in a nonsinusoidal shape of $I(\varphi)$ due to shift of Andreev bound states. Similar situation occurs in long SFS junctions with ideally transparent interfaces in the clean [17] and diffusive [7, 8] regimes. However, in the latter case the effects take

place only in a narrow interval of very low temperatures (due to smallness of the Thouless energy), while here we shall consider short-length structures where the effects are more pronounced and exist practically in the whole temperature range (the role of temperature will be discussed elsewhere [18]).

In this letter we investigate anomalies of the $I(\varphi)$ relation in several types of SFS structures which allow analytical solution while have not been fully explored yet: the SFcFS point contact with clean or diffusive constriction as a weak link, and the double-barrier SIFS junction; the ferromagnetic layers are assumed to be thin, and the magnetization is homogeneous throughout the F part of the system. In particular, we show that the maximum of $I(\varphi)$ can shift from $\pi/2 \leq \varphi_{\max} < \pi$ to $0 < \varphi_{\max} < \pi/2$ as a function of the exchange field in the ferromagnet. Previously, current–phase relation of this type was theoretically predicted either if superconductivity in the S-electrodes was suppressed by the supercurrent in the SNS structure [19, 20, 21] or in the vicinity of $T = 0$ in long SFS junctions [7, 8].

The outline of the paper is as follows. We start with studying the SFcFS structure composed of two SF sandwiches linked by a clean Sharvin constriction with arbitrary transparency D . We show that the energy–phase relation of this junction can have *two* minima: at $\varphi = 0$ and $\varphi = \pi$ (while the energy of the junction in the pure 0- or π -state has a *single* minimum — at $\varphi = 0$ or $\varphi = \pi$, respectively). As a result, $I(\varphi)$ dependence can intersect zero not only at $\varphi = 0$ and $\varphi = \pi$ but also at an arbitrary value φ_0 from the interval $0 < \varphi_0 < \pi$. The salient effects which occur in junctions with clean constriction survive averaging over the distribution of transmission eigenvalues and thus occur also in diffusive point contacts. Physically, the properties of SFS struc-

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tures are explained by splitting of Andreev levels due to the exchange field; to demonstrate this, we study the spectral supercurrent. Finally, we show that the same mechanism provides shifting of the $I(\varphi)$ maximum to $\varphi < \pi/2$ in the double-barrier SIFIS junctions which can be more easily realized in experiment.

SFcFS with clean constriction. We start with a model structure composed of two superconducting SF bilayers connected by a clean constriction with transparency D (the size of the constriction a is much smaller than the mean free path l : $a \ll l$). We assume that the S-layers are bulk and that the dirty limit conditions are fulfilled in the S- and F-metals. For simplicity we also assume that the parameters of the SF interfaces γ and γ_B obey the condition

$$\gamma \ll \max(1, \gamma_B), \quad (1)$$

$$\gamma_B = R_B \mathcal{A}_B / \rho_F \xi_F, \quad \gamma = \rho_S \xi_S / \rho_F \xi_F,$$

where R_B and \mathcal{A}_B are the resistance and the area of the SF interfaces; $\rho_{S(F)}$ is the resistivity of the S (F) material, and the coherence lengths are related to the diffusion constants $D_{S(F)}$ as $\xi_{S(F)} = \sqrt{D_{S(F)}/2\pi T_c}$, where T_c is the critical temperature of the S-material. We shall consider symmetric structure and restrict ourselves to the limit when the thickness of the F-layers is small:

$$d_F \ll \min(\xi_F, \sqrt{D_F/2H}), \quad (2)$$

where H is the exchange energy in the F-layers.

Under condition (1), we can neglect the suppression of superconductivity in the S-electrodes by the supercurrent and the proximity effect, and reduce the problem to solving the Usadel equations [22] in the F-layers

$$\xi_F^2 \frac{\partial}{\partial x} \left[G_F^2 \frac{\partial}{\partial x} \Phi_F \right] - \frac{\tilde{\omega}}{\pi T_c} G_F \Phi_F = 0, \quad (3)$$

with the boundary conditions at the SF interfaces ($x = \mp d_F$) in the form [23]

$$\pm \gamma_B \frac{\xi_F G_F}{\tilde{\omega}} \frac{\partial}{\partial x} \Phi_F = G_S \left(\frac{\Phi_F}{\tilde{\omega}} - \frac{\Phi_S}{\omega} \right), \quad (4)$$

$$G_S = \omega / \sqrt{\omega^2 + \Delta_0^2}, \quad \Phi_S(\mp d_F) = \Delta_0 \exp(\mp i\varphi/2).$$

In the above equations the x axis is perpendicular to the interfaces with the origin at the constriction; $\omega = \pi T(2n+1)$ are Matsubara frequencies; $\tilde{\omega} = \omega + iH$; and Δ_0 is the absolute value of the pair potential in the superconductors. The function Φ parameterizes the Usadel functions G , F , and \bar{F} :

$$G_F(\omega) = \frac{\tilde{\omega}}{\sqrt{\tilde{\omega}^2 + \Phi_F(\omega)\Phi_F^*(-\omega)}}, \quad (5)$$

$$F_F(\omega) = \frac{\Phi_F(\omega)}{\sqrt{\tilde{\omega}^2 + \Phi_F(\omega)\Phi_F^*(-\omega)}}, \quad \bar{F}_F(\omega) = F_F^*(-\omega).$$

Under condition (2), the spatial gradients in the F-layers arising due to the proximity effect and current are small. Then we can expand the solution of Eqs. (3)–(5) up to the second order in small gradients, arriving at [12]

$$\Phi_{F1, F2} = \Phi_0 \exp(\mp i\varphi/2), \quad \Phi_0 = \Delta_0 \tilde{\omega}/W, \quad (6)$$

where

$$W = \omega + \tilde{\omega} \gamma_{BM} \Omega, \quad \Omega = \sqrt{\omega^2 + \Delta_0^2} / \pi T_c, \quad (7)$$

$$\gamma_{BM} = \gamma_B d_F / \xi_F,$$

and the indices 1 and 2 refer to the left- and right-hand side of the constriction, respectively.

The supercurrent in constriction geometry is given by the general expression [24]

$$I = \frac{4\pi T}{e R_N} \text{Im} \sum_{\omega > 0} \frac{(\bar{F}_1 F_2 - F_1 \bar{F}_2)/2}{2 - D [1 - G_1 G_2 - (\bar{F}_1 F_2 + F_1 \bar{F}_2)/2]}, \quad (8)$$

where R_N is the normal-state resistance of the junction. Inserting Eq. (6) in this expression we obtain

$$I = \frac{2\pi T}{e R_N} \text{Re} \sum_{\omega > 0} \frac{\Delta_0^2 \sin \varphi}{W^2 + \Delta_0^2 [1 - D \sin^2(\varphi/2)]}. \quad (9)$$

Finally, the current–phase relation takes the form

$$I(\varphi) = \frac{2\pi T}{e R_N} \sum_{\omega > 0} \frac{A \Delta_0^2 \sin \varphi}{A^2 + B^2}, \quad (10)$$

$$A = \Delta_0^2 [1 - D \sin^2(\varphi/2)] - H^2 (\gamma_{BM} \Omega)^2 + \omega^2 (1 + \gamma_{BM} \Omega)^2,$$

$$B = 2\omega H \gamma_{BM} \Omega (1 + \gamma_{BM} \Omega).$$

At small ω the function A [and thus $I(\varphi)$] changes its sign at finite phase difference $\varphi_c = 2 \arcsin \sqrt{[1 - (\gamma_{BM} h)^2]/D}$ if the exchange field is in the range $1 - D < (\gamma_{BM} h)^2 < 1$; here h is the normalized exchange field, $h = H/\pi T_c$. The results for $I(\varphi)$ are shown in Figs.1,2 and can be understood by considering the spectral supercurrent density $\text{Im} J(\varepsilon)$. The latter is obtained by the analytical continuation in Eq. (9) and is given by a sum of delta-functions $\delta(\varepsilon - E_B)$ where E_B are energies of the Andreev bound states. At $\gamma_{BM} = 0$ the well-known result $E_B = \pm \Delta_0 \sqrt{1 - D \sin^2(\varphi/2)}$ is reproduced, while at finite γ_{BM} the exchange field splits each bound state into two (see inset in Fig.1). At $\varphi = \varphi_c$ one of these split (positive) peaks crosses zero leaving the domain $\varepsilon > 0$, and simultaneously a negative peak moves from

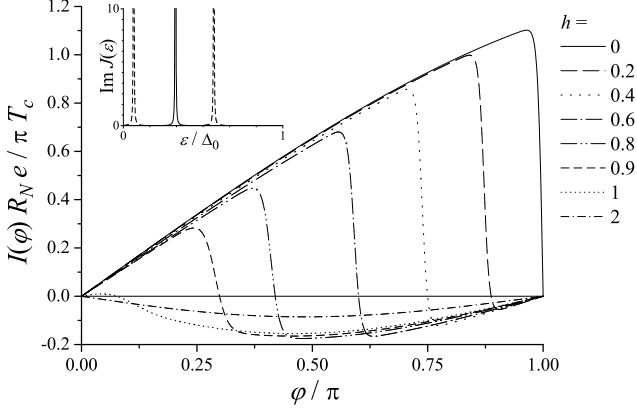


Fig.1. Current–phase relation in clean SFcFS junction with ideally transparent constriction ($D = 1$) at $T/T_c = 0.01$, $\gamma_{BM} = 1$ for different values of the normalized exchange field h . Inset: spectral supercurrent density at $\varphi = 2\pi/3$ for $h = 0$ (solid line) and $h = 0.4$ (dashed line).

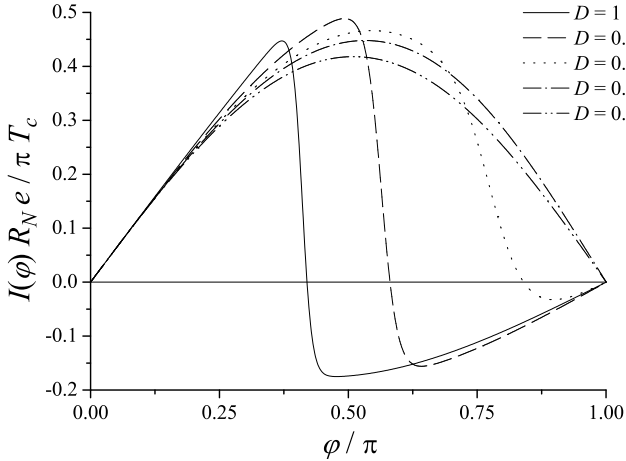


Fig.2. Current–phase relation in clean SFcFS junction at $T/T_c = 0.01$, $\gamma_{BM} = 1$, $h = 0.8$ for different values of the barrier transparency D .

the region $\varepsilon < 0$ into $\varepsilon > 0$ reversing the sign of the supercurrent.

The sign-reversal of the supercurrent (the $0-\pi$ transition) can also be achieved at *fixed* H due to nonequilibrium population of levels. This phenomenon has been studied in long diffusive SNS [25, 26, 27] and SFS junctions [7, 8].

SFcFS with diffusive constriction. To get the $I(\varphi)$ relation for the diffusive point contact [$l \ll a \ll \min(\xi_F, \sqrt{D_F/2H})$] we integrate $\int_0^1 \rho(D)I(D)dD$, where $I(D)$ is given by Eq. (9) for the clean case (note that $R_N \propto D^{-1}$ in this equation) and $\rho(D)$ is

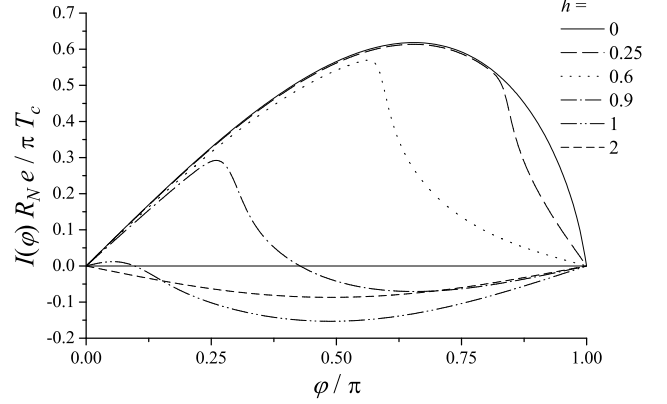


Fig.3. Current–phase relation in diffusive SFcFS point contact at $T/T_c = 0.01$, $\gamma_{BM} = 1$ for different values of the exchange field h .

Dorokhov's density function $\rho(D) = 1/2D\sqrt{1-D}$ [28]. Finally, we arrive at the result

$$I(\varphi) = \frac{4\pi T}{eR_N} \text{Re} \sum_{\omega>0} \frac{\Delta_0 \cos(\varphi/2)}{\sqrt{W^2 + \Delta_0^2 \cos^2(\varphi/2)}} \times \arctan \left(\frac{\Delta_0 \sin(\varphi/2)}{\sqrt{W^2 + \Delta_0^2 \cos^2(\varphi/2)}} \right). \quad (11)$$

This expression coincides with the direct solution of the Usadel equations, and at $\gamma_{BM} = 0$ it reproduces the Kulik–Omelyanchuk formula for the diffusive ScS constriction [29].

Calculation of $I(\varphi)$ using the above expression yields results similar to those for the clean point contact, however the transition from 0- to π -state becomes less sharp (see Fig.3).

Temperature dependence of the critical current in this case shows thermally-induced $0-\pi$ crossover with nonzero critical current at the transition point, in agreement with results of Refs. [8, 10] (results for $I_c(T)$ will be presented elsewhere [18]). This is a natural result since the barrier transparency is high and the current–phase relation is strongly nonsinusoidal. We note that in Ref. [13] the measured critical current vanished at the $0-\pi$ transition point because of the low transparency regime (and hence sinusoidal current–phase relation) realized in that experiment.

SIFIS. Now we turn to a double-barrier SIFIS junction (I denotes an insulating barrier) — this structure is easier for experimental implementation than an SFcFS junction. In the case of SIFIS, due to dephasing effects (this situation is similar to the SINIS junction [30]) the supercurrent can not be derived by integrating over the corresponding transmission distribution (except for the

case of vanishing γ_{BM}) and must be calculated by solving the Usadel equations.

We assume that condition (1) is satisfied; then we can neglect the suppression of superconductivity in the S-electrodes by the supercurrent and the proximity effect. In this case the system is described by Eqs. (3)–(5), although now instead of two F-layers connected by a constriction we have a continuous F-layer (at $-d_F < x < d_F$).

We also assume that the F-layer is thin [condition (2)] and that $\gamma_B \gg d_F/\xi_F$, hence the spatial gradients in the F-layer are small. Then (similarly to the case of constriction) we can expand the solution of Eqs. (3)–(5) up to the second order in small gradients, arriving at

$$\Phi_F = \Phi_0 \cos(\varphi/2) + i \frac{\tilde{\omega} G_S}{\omega G_F} \frac{\Delta_0 \sin(\varphi/2)}{\gamma_B} \frac{x}{\xi_F}, \quad (12)$$

$$G_F = \frac{\tilde{\omega}}{\sqrt{\tilde{\omega}^2 + \Phi_0^2 \cos^2(\varphi/2)}}, \quad (13)$$

with Φ_0 defined in Eq. (6) [in the final result (12) we retained only the first order in gradients — this accuracy is sufficient for calculating the current].

Inserting the solution (12), (13) into the general expression for the supercurrent

$$I = -\frac{\pi T \mathcal{A}_B}{e \rho_F} \text{Im} \sum_{\omega} \frac{G_F^2(\omega)}{\tilde{\omega}^2} \Phi_F(\omega) \frac{\partial}{\partial x} \Phi_F^*(-\omega), \quad (14)$$

we obtain

$$I(\varphi) = \frac{2\pi T}{e R_N} \text{Re} \sum_{\omega > 0} \frac{\Delta_0^2 \sin \varphi}{\sqrt{\omega^2 + \Delta_0^2} \sqrt{W^2 + \Delta_0^2 \cos^2(\varphi/2)}} \quad (15)$$

(our assumptions imply that $R_N \approx 2R_B$). This result demonstrates that the SIFIS junction with thin F-layer is always in the 0-state.²⁾ Nevertheless, $I(\varphi)$ is strongly modified by finite H (see Fig.4), especially at small temperatures. Figure 4 clearly demonstrates that an increase of H results not only in suppression of the critical current, but also in the shift of the $I(\varphi)$ maximum from $\varphi_{\max} \approx 1.86$ at $H = 0$ to the values smaller than $\pi/2$. In the limit of large exchange fields, $h \gg \gamma_{BM}^{-1}$, $I(\varphi)$ returns to the sinusoidal form.

²⁾In the case under discussion when the F-layers are thin and the interface parameters obey condition (1), the phase of the pair potential is constant in the S-part and almost constant in the F-part, however it jumps at the two SF interfaces [12]. The two jumps compensate each other in SIFIS with a single F-layer, whereas in SFcFS they add up at the weak link thus opening possibility for the π -state.

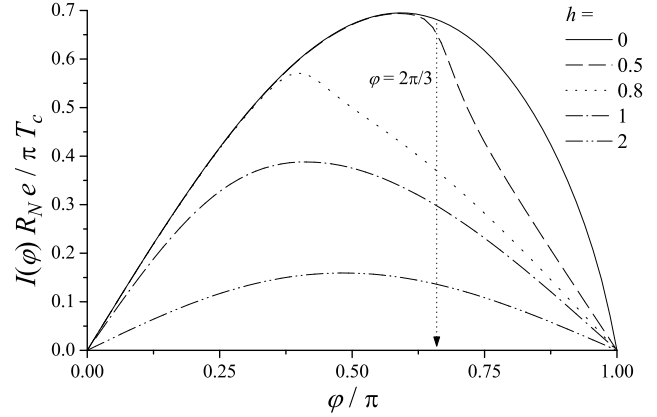


Fig.4. Current–phase relation in double-barrier SIFIS junction at $T/T_c = 0.02$, $\gamma_{BM} = 1$ for different values of the exchange field h . The value $\varphi = 2\pi/3$ will be used in Fig.5.

The physical origin of these results can be clarified in the real energy ε representation. Making analytical continuation in Eq. (15) by replacement $\omega \rightarrow -i(\varepsilon + i0)$, we obtain the spectral supercurrent density $\text{Im} J(\varepsilon)$ which contains contributions of Andreev bound states with different energies:

$$I = \frac{1}{4eR_N} \sum_{\sigma=\pm 1} \int \text{Im} J(\varepsilon, \sigma H) \tanh\left(\frac{\varepsilon}{2T}\right) d\varepsilon, \quad (16)$$

$$\text{Im} J(\varepsilon, H) = \text{Im} \frac{\Delta_0^2 \sin \varphi}{\sqrt{\Delta_0^2 - \varepsilon^2} \sqrt{\Delta_0^2 \cos^2(\varphi/2) - \tilde{\varepsilon}^2}}, \quad (17)$$

$$\tilde{\varepsilon} = \varepsilon + \gamma_{BM}(\varepsilon - H)\Omega(\varepsilon), \quad \Omega(\varepsilon) = \sqrt{\Delta_0^2 - \varepsilon^2}/\pi T_c.$$

Equation (17) implies that at $\varphi_c = 2 \arccos(\gamma_{BM} h)$ singularities in $\text{Im} J(\varepsilon)$ are shifted to the Fermi level. At $\varphi > \varphi_c$ the negative singularity in $\text{Im} J(\varepsilon)$ for one spin projection crosses the Fermi level and appears in the positive energy domain, whereas the positive peak for the other projection leaves the domain $\varepsilon > 0$ (this process is illustrated in Fig.5). As a result, the contribution to the supercurrent from low energies changes its sign, and the supercurrent $I(\varphi)$ becomes suppressed at $\varphi > \varphi_c$ (see Fig.4). However, at higher energies $\varepsilon \sim \Delta_0$ modifications in $\text{Im} J(\varepsilon)$ are weak, and the resulting $I(\varphi)$ does not change its sign.

In conclusion, we have studied nonsinusoidal current–phase relation in Josephson junctions with thin ferromagnetic interlayers and identified the physical mechanisms of these effects in terms of splitting of Andreev bound states in the junction by the exchange field. In particular, we have shown that zero-energy crossing of Andreev bound states is responsible for the sign-reversal of $I(\varphi)$, which also survives averaging over distribution of transmission eigenvalues in the diffusive

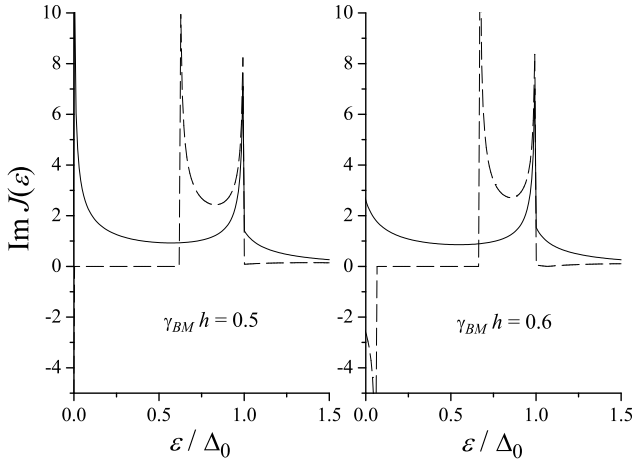


Fig.5. Spectral supercurrent in diffusive double-barrier SIFS junction with thin ferromagnetic interlayer at $\gamma_{BM} = 1$, $\varphi = 2\pi/3$ for two values of the exchange field h . The chosen value of φ corresponds to φ_c at $\gamma_{BM}h = 0.5$, and the figure demonstrates that the positive peak for one spin projection disappears from while the negative peak for the other projection appears in the domain $\varepsilon > 0$.

junction. As a result, the energy–phase relation for the junction has two minima: at $\varphi = 0$ and $\varphi = \pi$. The phenomena studied in this work may be used for engineering cryoelectronic devices manipulating spin-polarized electrons and in qubit circuits.

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